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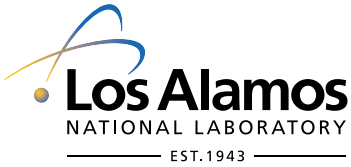

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Review of the Forest Fire Model

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September 17, 2006

Abstract

The Forest Fire burn model is used in reactive hydro simulations to describe both initiation and propagation of a detonation wave. Here we thoroughly review the assumptions of the model, provide a derivation of the Forest fire rate based on characteristics in analogy with Whitham-Chisnell shock dynamics, and discuss issues with code implementation.

1 Introduction

Detonation wave phenomena are simulated using the reactive Euler equations.

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u\\ \rho E\\ \rho\lambda\end{pmatrix}+\frac{\partial}{\partial x}\begin{pmatrix}\rho u\\ \rho u^2+P\\ \rho u(E+PV)\\ \rho u\lambda\end{pmatrix}=\begin{pmatrix}0\\ 0\\ 0\\ \rho\,\mathcal{R}\end{pmatrix}\ , \tag{1}$$

where ρ is the density, $V=1/\rho$ is the specific volume, $E=e+\frac{1}{2}u^2$ is the total specific energy, e is specific internal energy, u is the particle velocity, P is the pressure, λ is the reaction progress variable and $\mathcal{R}$ is the reaction rate. A high explosive (HE) is assumed to be a mixture of reactants and

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products with λ the mass fraction of the products. Moreover, it is assumed that partly burned HE can be characterized by a mixture equation of state (EOS), $P(V, e, \lambda)$. Furthermore, e is assumed to include the chemical energy. Therefore, the EOS accounts for energy released in the reaction and there is no source term in the equation for conservation of energy.

Solid explosives are heterogeneous and have different detonation properties than gaseous and liquid explosives which are homogeneous; see [Campbell et al., 1961a,b]. Forest fire[1] is one of the first burn models aimed at describing solid explosives. Though the HE is treated as homogeneous, an "effective" burn rate, rather than a chemical rate, is used to account for reaction due to unresolved hot spots that arise when a heterogeneous explosive is subjected to a strong compressive wave. The model has been widely applied to applications involving initiation and propagation of detonation waves in plastic-bonded explosives (PBX); see [Mader, 1998] and references therein.

The reaction rate for the Forest fire model is assumed to have the form

$$\mathcal{R} = (1 - \lambda)\mathcal{R}_{\text{FF}}(P) \ . \tag{2}$$

The depletion factor, $1-\lambda$, corresponds to a first order reaction. The function $\mathcal{R}_{\text{FF}}(P)$ is fit to shock-to-detonation transition data; see [Mader and Forest, 1976], [Mader, 1998, sec. 4.1]. The purpose of this article is to review the assumptions that go into the derivation of the Forest fire rate, and to discuss some of the issues with its implementation and use.

The assumptions of the model are stated and discussed in sec. 2. The reactive shock Hugoniot and Pop-plot[2] data play a key role in the derivation of the Forest fire rate. The reactive locus is described in sec. 3. Typically, the locus is specified by giving the shock velocity as a function of particle velocity. A derivation is given for the burn fraction behind a reactive shock. Next, in sec. 4, the Pop plot and the wedge experiment, on which it is based, are described. Then a derivation of the Forest fire rate, based on characteristics, is presented in sec. 5 along with an analogy to Whitham-Chisnell shock dynamics. Issues with implementing the Forest fire model in a hydro code are discussed in sec. 6. The most important is the treatment of a reactive shock within the context of a shock capturing algorithm. To illustrate the behavior of the Forest fire model, numerical results for a shock-to-detonation transition are shown in sec. 7. Simplified burn models, such

[1]Named after its originator Charles Forest.

[2]Named after its originator Alphonse Popolato.

as Forest fire, have generic limitations associated with shock desensitization and the curvature effect. These are briefly discussed in sec. 8. Concluding remarks, related to the effectiveness of the model, are presented in sec. 9.

2 Model assumptions

The Forest fire model has been developed and calibrated for plastic-bonded explosives. These consist of explosive grains held together by a polymeric binder. The cell size for reactive hydro simulations is typically much greater than the size of an average grain. Consequently, a homogenized model is used for the explosive. In addition, a single-step reaction is assumed; reactants to products.

We note that some PBX formulations, such as PBX 9404, use an energetic binder. Moreover, it is known that some explosives, such as TATB, have both fast and slow reactions. Thus, the assumption of a single-step reaction is a crude approximation used to simplify modeling of an HE.

The pressure behind a detonation wave is much higher than the yield strength of the explosive grains. Consequently, for the detonation regime, it is a reasonable approximation to neglect material strength and treat the reactants as a fluid. The material properties of both the reactants and the products are characterized by an EOS. Partly burned HE is assumed to be described by a mixture EOS, $P(V, e, \lambda)$, which interpolates between the reactants ($\lambda = 0$) and the products ($\lambda = 1$) equations of state.

The Forest fire model is based on three further assumptions; pressure-temperature equilibrium for partly burned HE, single curve buildup principle, and a pressure dependent fitting form for the burn rate. We discuss each of these assumptions in turn.

2.1 Pressure-temperature equilibrium

A mixture EOS requires a closure assumption. If burn is volumetric in nature, reactants and products would be well mixed. Then it is reasonable to treat partly burned HE in pressure-temperature equilibrium.

Let subscript '1' denote the reactants and subscript '2' denote the products. Thus, the mass fraction of the reactants is $\lambda_1 = 1 - \lambda$, and the mass fraction of the products is $\lambda_2 = \lambda$. The pressure-temperature equilibrium

equation of state, $P(V, e, \lambda)$, is determined by the equations

$$\begin{aligned} V &= \lambda_1 V_1 + \lambda_2 V_2 \ , \\ e &= \lambda_1 e_1 + \lambda_2 e_2 \ , \\ P &= P_1(V_1, e_1) = P_2(V_2, e_2) \ , \\ T &= T_1(V_1, e_1) = T_2(V_2, e_2) \ . \end{aligned} \tag{3}$$

If the component EOS are thermodynamically consistent,[3] then it can be shown that Eq. (3) has a unique solution, provided that the domain of the components include the (P, T) regime of interest. Moreover, the mixture EOS is thermodynamically consistent. Hence, the mixture sound speed is well defined, and Eq. (1) maintains the usual hyperbolic properties of the Euler equations.

Numerically, a pressure-temperature equilibrium EOS is computed with an iterative algorithm to solve Eq. (3). Many algorithms restrict the component EOS such that the specific heat, $C_V = \partial_T e|_V$, is constant and the Grüneisen coefficient, $\Gamma = V\partial_e P|_v$, is a function of only V. Due care is needed to ensure that each iteration is within the domain of the component EOS and that the iterations converge. Because of the reactive source terms, simulations are much more sensitive to numerical errors in evaluating the mixture EOS for an explosive than for inert materials.

Based on the physical processes that take place at the mesoscale, other closure assumptions are possible. Reaction in a heterogeneous explosive is due to hot spots or localized regions of high temperature. Suppose a hot spot reacts on a short temporal scale and gives rise to a deflagration front. This is the underlying physical picture behind the ignition and growth model of Lee and Tarver [1980]. Across the front, the reactants and products are in neither pressure nor temperature equilibrium. Typically, the pressure jump across a deflagration front is small. However, at the Chapman-Jouguet (CJ) pressure the deflagration speed can be a significant fraction of the detonation speed [Esposito et al., 2003]. Since $\Delta P/\Delta V = -(\rho D)^2$, the pressure jump across a deflagration front may not be negligible.

A non-equilibrium treatment would require a two-phase fluid model in order to tract the specific energy and specific volume separately for the reactants and products. One possibility for a mixture rule is to track the shock

[3] P and T derivable from a thermodynamic potential (such as the Helmholtz free energy), the specific heat $C_V = \partial_T e|_V > 0$, and the isothermal sound speed squared $c_T^2 = -V^2 \partial_V P|_T > 0$.

pressure and replace temperature equilibrium condition with the condition that the reactants are on the isentrope of the shock state; see [Johnson et al., 1985]. Another mixture rule assumes that the pressure is a weighted average of the component pressures;

$$P(V, e) = \lambda_1 P_1(V, e) + \lambda_2 P_2(V, e) \ .$$

Simple ad hoc closure assumptions run the risk of a thermodynamic inconsistent mixture EOS and unphysical behavior for solutions to the reactive Euler equations.

2.2 Single curve buildup principle

Shock ignition of heterogeneous explosives have been studied by measuring the x–t trajectory of the lead front; see Campbell et al. [1961a]. The transition to a detonation wave is very abrupt. Consequently, trajectories for different initiation pressures can be compared by shifting the (x, t) origin to correspond to the transition point[4]. It is then observed that the measured trajectories lie on top of each other. This led to the hypothesis that the x–t trajectory for a shock-to-detonation transition is independent of the starting pressure; see [Mader, 1965, App. D, p. 119]. The hypothesis is known as the *single curve buildup principle*.

The most careful test of the principle has been performed on an RDX based PBX by Linstrom [1966]. Within the uncertainties in the measurements, Lindstrom found that a single trajectory is consistent with the RDX data. Another study by Dick [1981] found reasonable but not perfect agreement among front trajectories for PBX 9404 and PBX 9502. However, Dick used unpublished data of other researchers and did not propagate uncertainties in the data through his analysis. Later, in subsection 5.1, based on an analogy with the Guderley solution for a converging shock, we suggest that the single curve buildup principle is an asymptotic property of shock-to-detonation solutions to the reactive Euler equations.

An important consequence of the single shock buildup principle is that shock ignition can be characterized by the run-to-detonation distance as a function of ignition pressure. Run distance versus pressure, on a log-log scale, is known as a *Pop plot*. This is discussed in more detail in sec. 4.

[4]The transition point is somewhat fuzzy as it can not be defined more accurately than the reaction zone width for a steady detonation wave. Typically, this uncertainty is small compared to the spatial interval over which a trajectory is measured.

2.2.1 Reactive Hugoniot

The same experiments that are used to determine the Pop plot also measure points on the Hugoniot locus. Early experiments on PBX 9404 indicated that in the (u_p, u_s)–plane, the locus is a straight line starting at $(0, c_0)$ and extrapolating to the CJ state; see [Ramsay and Popolato, 1965, fig. 2]. This led to the further hypothesis that the lead front in a shock-to-detonation transition is a reactive shock; see [Ramsay and Popolato, 1965] and [Mader, 1970]. Other Hugoniot data for PBX 9404 [Gibbs and Popolato, 1980, pp. 359–362] do not extrapolate to the CJ state. Nevertheless, the derivation of the Forest fire model utilizes the reactive shock hypothesis.

The ambiguity of whether or not the lead front is a reactive shock, occurs because of the difficulty in measuring the shock state for a HE. The shock state is inferred from a measurement of the shock velocity. Typically, shock velocity is determined by the transit time for a given distance of run. If the transit time is not sufficiently small then the reaction over the measurement interval may be significant. Thus, limited spatial and temporal resolution can result in a systematic error corresponding to a reactive shock.

2.3 Pressure dependent rate

The Forest fire model assumes that the reaction rate is pressure dependent, Eq. (2). Moreover, the rate function, $\mathcal{R}_{\text{FF}}(P)$, is fit to the rate behind a reactive shock. The essence of the Forest fire model is the determination of the rate behind a reactive shock based on the single curve buildup principle and the assumption that gradients behind the shock front can be neglected. A derivation is given in a later section.

The reactive shock locus can be parameterized by a single thermodynamic variable. The choice of pressure to parameterize the shock locus and hence the reactive rate, enables the model to be well behaved in numerical simulations. Acoustic waves provide a feedback mechanism that corrects local numerical errors in the pressure. In contrast, numerical errors in entropy are persistent, and affect both the density and temperature.

Plastic-bonded explosives have a small amount of porosity. The ignition sensitivity of a PBX increases with porosity. One mechanism for generating hot spots is based on pore collapse; see for example [Mader, 1965] and [Menikoff, 2004]. Therefore, it is plausible that shock pressure is the driving force that activates hot spots. Consequently it is reasonable that the effective

reaction rate would be dominated by pressure.

3 Reactive Hugoniot locus

A partly burned Hugoniot locus, with fixed burn fraction λ, is defined by the Hugoniot equation

$$e_1 = e_0 + \tfrac{1}{2}(P_1 + P_0)(V_0 - V_1) \ , \tag{4}$$

where $P_1 = P(V_1, e_1, \lambda)$. As λ increases these loci interpolate from the reactant Hugoniot locus ($\lambda = 0$) to the product detonation locus ($\lambda = 1$). The mixture EOS is assumed to satisfy the condition that the pressure increases with burn fraction; $\partial_\lambda P > 0$. It can then be shown that the loci in the (V, P)–plane with different values of λ do not cross.

A reactive Hugoniot locus can be specified by a u_s–u_p relation for the shock velocity as a function of particle velocity; $u_s(u)$. The intersection in the (V, P)–plane of the Rayleigh line with slope $-(\rho_0\, u_s)^2$ and the line $P =$ constant coincides with a unique partly burned Hugoniot locus. This determines the value of λ on a reactive shock.

The partly burned Hugoniot loci have a subsonic (strong) branch and a supersonic (weak) branch. The two branches meet at a sonic point, which we refer to as the CJ state for a partly burned locus. We require that a partly burned reactive shock to be on the subsonic branch; *i.e.*, $u + c > u_s$. The frozen sound speed, c, is determined from the EOS by

$$(\rho\, c)^2 = -\partial_V P + P\partial_e P \ ,$$

where the partial derivatives are at fixed λ.

The value of λ on the reactive Hugoniot locus can also be found from an ODE. It is convenient to parameterize the reactive locus by u. In terms of the mixture EOS, the shock pressure can be expressed as

$$P_s(u) = P\Big(V(u), e(u), \lambda(u)\Big) \ .$$

Then by taking derivative of the shock pressure, one obtains

$$\frac{\mathsf{d}\lambda}{\mathsf{d}u} = \frac{\frac{\mathsf{d}P}{\mathsf{d}u} - (\partial_V P)\frac{\mathsf{d}V}{\mathsf{d}u} - (\partial_e P)\frac{\mathsf{d}e}{\mathsf{d}u}}{\partial_\lambda P} \ , \tag{5}$$

where the partial derivatives are based on the mixture EOS, and $\frac{\mathsf{d}}{\mathsf{d}u}$ is the derivative along the Hugoniot locus.

To determine $\partial_\lambda P$ consider the reactants and products variables to be functions of λ; *i.e.*, $V_i(\lambda)$, $e_i(\lambda)$ for $i = 1, 2$. Taking $\mathsf{d}/\mathsf{d}\lambda$ of Eq. (3) leads to a system of 4 simultaneous equations for $\mathsf{d}V_i/\mathsf{d}\lambda$ and $\mathsf{d}e_i/\mathsf{d}\lambda$. Then $\partial_\lambda P = (\partial_V P_1)\mathsf{d}V_1/\mathsf{d}\lambda + (\partial_e P_1)\mathsf{d}e_1/\mathsf{d}\lambda$. The other two quantities, $\partial_V P$ and $\partial_e P$, can be determined in a similar manner.

From the shock jump relations

$$
\begin{aligned}
V(u) &= \left[1 - \frac{u}{u_s}\right] V_0 \ , \\
e(u) &= e_0 + P_0\, V_0 \left[\frac{u}{u_s}\right] + 0.5\, u^2 \ , \\
P(u) &= P_0 + \rho_0\, u\, u_s \ ,
\end{aligned}
$$

we obtain

$$
\frac{\mathsf{d}V}{\mathsf{d}u} = -\left[1 - \frac{u}{u_s}\,\frac{\mathsf{d}u_s}{\mathsf{d}u}\right]\frac{V_0}{u_s} \ , \tag{6a}
$$

$$
\frac{\mathsf{d}e}{\mathsf{d}u} = u + \left[1 - \frac{u}{u_s}\,\frac{\mathsf{d}u_s}{\mathsf{d}u}\right]\frac{P_0\, V_0}{u_s} \ , \tag{6b}
$$

$$
\frac{\mathsf{d}P}{\mathsf{d}u} = \left[1 + \frac{u}{u_s}\,\frac{\mathsf{d}u_s}{\mathsf{d}u}\right]\rho_0 u_s \ . \tag{6c}
$$

The ODE, Eq. (5), is closed by specifying a u_s–u_p relation for the reactive Hugoniot locus. Typically, it is assumed that $u_s(u)$ is a linear function from the initial state to the CJ state; $u_s = c_0 + s\, u$. In this simple case, $\frac{\mathsf{d}u_s}{\mathsf{d}u} = s = (D_{\mathrm{CJ}} - c_0)/u_{\mathrm{CJ}}$, where D_{CJ} is the detonation speed and u_{CJ} is the particle velocity at the CJ state.

3.1 Example — PBX 9501

Example reactive and partly burned Hugoniot loci are shown in fig. 1. The loci are calculated from an EOS for PBX 9501. The reactants EOS is based on Birch-Murnaghan form for the cold curve fit to HMX isothermal compression data [Menikoff and Sewell, 2004] with the initial density and sound speed adjusted to match PBX 9501. Analogous to the Debye model, C_V is

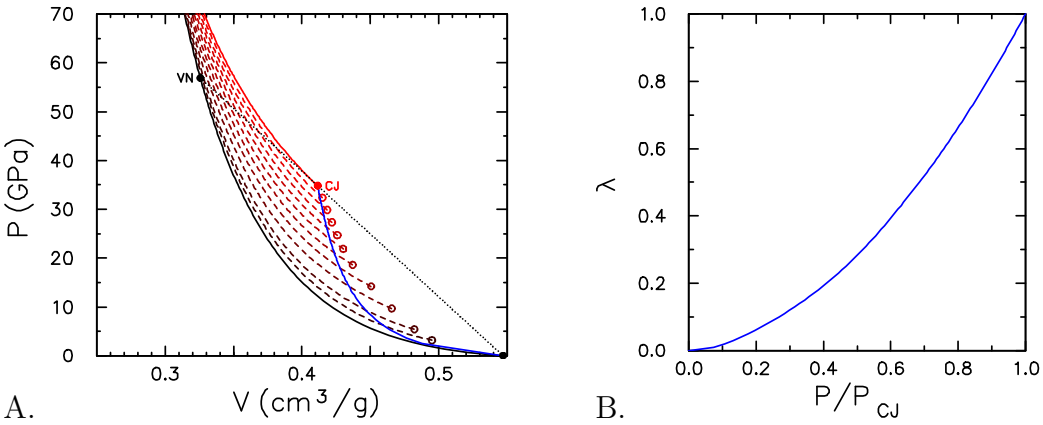


Figure 1: Hugoniot loci for PBX 9501. A. Partly burned and reactive loci in (V, P)–plane. Black curve is reactant locus ($\lambda = 0$) and red curve is product detonation locus ($\lambda = 1$). CJ states are indicated by open circles. Blue curve is reactive locus based on linear u_s–u_p relation. Dotted black line is Rayleigh line through CJ state. B. Reaction progress variable as function of pressure along reactive locus.

taken to be a function of a scaled temperature, $T/\theta(V)$, where the Grüneisen coefficient is given by $\Gamma(V) = -\mathsf{d}\ln(\theta)/\mathsf{d}\ln(V)$. At the initial density, the temperature dependence of C_V is fit to molecular dynamics calculations of Goddard et al. [1998, fig. 4.13]. A tabular Sesame EOS is used for the reactants. The table generated by Shaw [2004] is based on PBX 9501 overdriven detonation wave data [Fritz et al., 1996] and release wave data [Hixson et al., 2000] for high pressures ($P > 20\,\mathrm{GPa}$) and cylinder and sandwich experiment data at lower pressures. In addition, the reactive Hugoniot locus is based on a linear u_s–u_p relation connecting the initial state to the CJ state.

4 Run to detonation

A shock-to-detonation transition is characterized, to a large extent, by the x–t trajectory of the lead front. Shock initiation trajectories for many explosives have been measured with wedge experiments; see [Campbell et al., 1961a] and [Gibbs and Popolato, 1980, part II, sec. 4.1]. Comparison of the trajectories for different initiation pressures led to the single curve buildup principle. A consequence of this principle is that shock initiation can be characterized by a Pop plot or run-to-detonation distance as a function of initiation pressure.

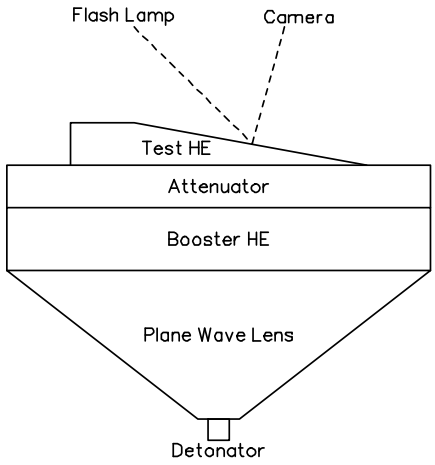


Figure 2: Schematic of wedge experiment.

The wedge experiments, which are the basis for the Pop plot, are described next.

4.1 Wedge experiment

For solid explosives, it is difficult to measure hydrodynamics quantities in the interior. The surface, however, is readily accessible to measurement. The wedge experiment is a clever design for measuring the trajectory of the lead front for a shock-to-detonation transition. The experimental configuration is shown in fig. 2. A planar shock wave from an explosive drive system is used to initiate a wedge shaped test sample of HE. The pressure of the initiation shock can be varied by adjusting the thickness of the attenuator and the selection of attenuator material or booster explosive.

Breakout of the reactive shock on the wedge surface changes its reflectivity. First motion of points along the wedge are recorded with a streak camera. Breakout of the shock also gives rise to a reflected rarefaction. However, because of the small wedge angle, the rarefaction does not influence the reactive front within the test HE. Hence the measured trajectory corresponds to the motion of a planar wave, *i.e.*, one-dimensional flow.

A typical x–t trajectory for a shock initiated detonation is shown in fig. 3. The transition to detonation is seen to be very abrupt. A less subjective and more accurate determination of the transition point can be made using a

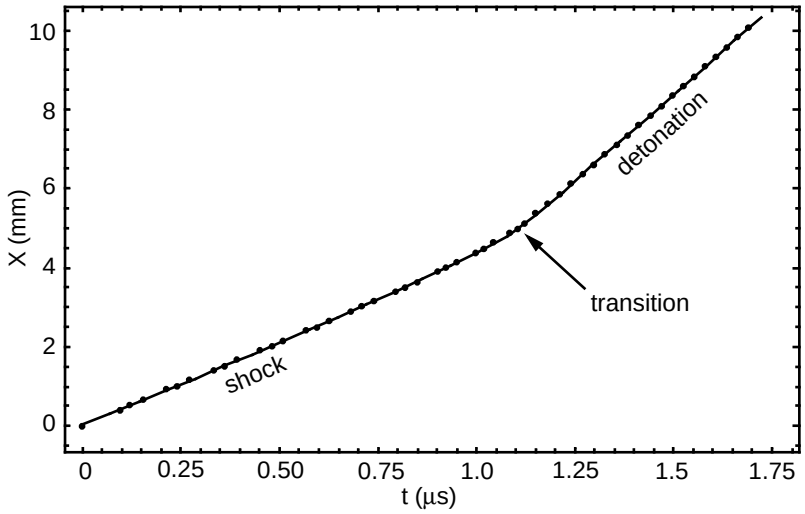


Figure 3: Front trajectory for shock-to-detonation transition in PBX 9501. Data points (dots) and fit (curve) are from Gustavsen et al. [1999, fig. 11]; reproduced with permission of the authors. Velocity gauge data for the same experiment is shown in fig. 9.

global fitting form for the trajectory data; see [Gustavsen et al., 1999] and [Hill and Gustavsen, 2002].

The data shown in fig. 3 is actual from an experiment that provides trajectory data equivalent to a wedge experiment but using a newer technique [Gustavsen et al., 1999]. Rather than an explosive drive system, the initiating shock is generated by the impact of a projectile launched by a gas gun. A magnetic tracker gauge is used to determine the front trajectory. In addition, magnetic velocity gauges measure Lagrangian time histories at a number of positions. Thus one experiment can provide data on the evolution of the velocity profile (see fig. 9) during a shock-to-detonation transition, as well as the front trajectory.

4.1.1 Initiation pressure

In addition to the front trajectory, one needs to know the initiation or drive pressure. This is determined as follows. Timing pins or other gauges are used to measure the free surface velocity of the attenuator. In conjunction with the EOS of the attenuator, the free surface velocity determines the incident

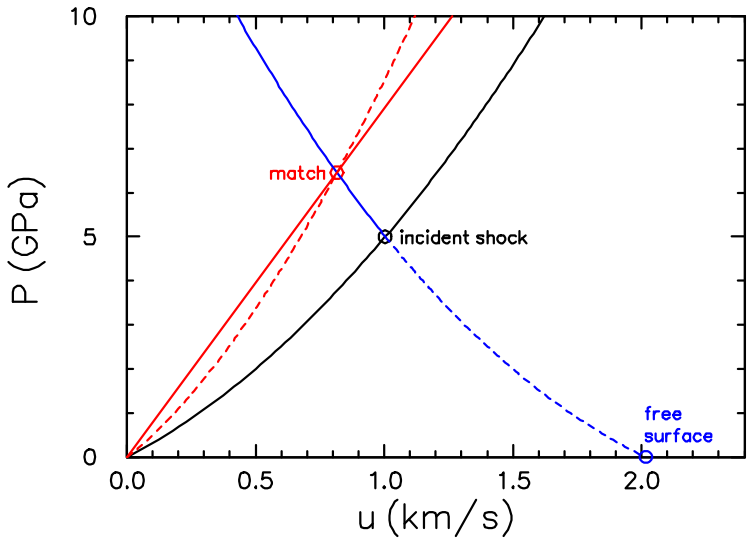


Figure 4: Example of graphical solution to impedance match for PMMA attenuator and PBX 9501 test HE. Black curve is incident Hugoniot locus for attenuator. Blue curve is reflected wave locus in attenuator; solid line is shock and dashed line is rarefaction. Solid red curve is Rayleigh line with slope $\rho_{\mathrm{HE}} u_s$. Dashed red curve is Hugoniot locus for the HE. The free surface velocity and incident shock in the attenuator are labeled. The match point corresponds to the initiation pressure for test HE in the wedge experiment.

shock strength in the attenuator. The initial slope of the x–t trajectory determines the initial shock velocity in the test HE. The intersection of the Rayleigh line with slope $\rho_{\mathrm{HE}} u_s$ and the reflected shock locus in the attenuator determines the initiation pressure for the test HE. The graphical construction is illustrated in fig. 4.

The impedance match for the drive pressure also determines a point on the Hugoniot locus of the test explosive. A leading source of uncertainty is the measurement of the initial shock velocity. The determination of the initial slope of the shock trajectory requires fitting data over an interval about the wedge tip. To facilitate construction the wedge tip may be truncated, thus blunting the sharp wedge angle. Consequently the initial shock velocity may actually correspond to the value after a small distance of run during which some reaction occurs. This resolution issue affects whether the Hugoniot locus is interpreted as reacted or unreacted.

Alternate techniques are now available to measure the unreacted shock Hugoniot [Sheffield et al., 2004]. These involve measuring time histories of the velocity at the HE interface. With a resolution of a few ns, one can distinguish the initial shock velocity from the subsequent change due to reaction. Also available are techniques for isentropic compression to high pressure. In a PBX, isentropic compression generates fewer and weaker hot spots than shock compression. Thus, the reactants EOS can be based on isentropic compression data rather than Hugoniot data; see [Hooks et al., 2006, Baer et al., 2006].

4.2 Pop plot

Distance-of-run to detonation can be fit to a straight line on a log-log plot [Ramsay and Popolato, 1965];

$$\log_{10}\Big((P - P_\star)/\mathrm{GPa}\Big) = a - b \times \log_{10}(x/\mathrm{mm}) \tag{7}$$

where $P_\star$ represents a pressure threshold. This is known as a Pop plot. The threshold pressure was added by Linstrom [1966] to achieve a better fit at low pressures to data on a RDX based PBX. Typically, wedge data does not extend to low pressures and the Pop plot is fit with $P_\star = 0$.

Wedge data for many explosives can be found in Gibbs and Popolato [1980, part II, sec. 4.1]. Example Pop plots are shown in fig. 5 for three explosives. PBX 9501 and PBX 9404 are both HMX based explosives. Their Pop plots show that the formulation of a PBX (binder and grain distribution) can affect the sensitivity, especially at low pressures. PBX 9502 is an insensitive explosive based on TATB. For a given pressure, it has larger distance of run than the more sensitive HMX based PBXs.

We note that data points from wedge experiments are usually limited to distances of run in the range of 1 to 20 mm. Difficulties occur for small run distances (high drive pressures) due to the accuracy at which the transition to detonation point on the x–t trajectory can be determined, and for large run distances (low drive pressures) due to rarefaction from the side of the wedge or pressure gradient in the drive system. With careful design and a large test sample, distance of run measurements can be extended up to 40 or 50 mm. Sensitive explosives require thick attenuators in the drive system and have a fairly uniform drive pressure. Measurements for insensitive explosives require thin attenuators and may be affected by pressure gradient from Taylor wave in the booster explosive.

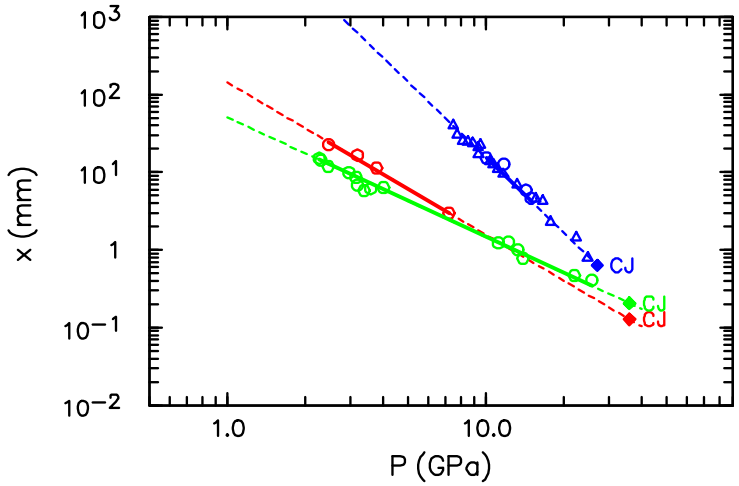


Figure 5: Example of Pop plots for three explosives. Red, green and blue lines are for PBX 9501, PBX 9404 and PBX 9502, respectively. Solid lines correspond to domain of fit to experimental data, and dashed lines are extrapolation. Solid diamonds are at CJ pressure of each explosive and circles denote data points. Fitting parameters and data points are from Gibbs and Popolato [1980]: PBX 9501, p. 115 and table 4.17; PBX 9404, p. 93 and table 4.18; PBX 9502, p. 126 and table 4.31. In addition, for PBX 9502, triangles are data points from [Dick et al., 1988, table I].

For the reactive shock model, in principle, distance-of-run to detonation goes to zero at the CJ pressure, *i.e.*, $x \to 0$ as $P \to P_{\rm CJ}$. It is noteworthy that the Pop plot extrapolated to CJ pressure gives a value for distance of run comparable to the reaction zone width. For example, distance of run for PBX 9501 extrapolated from the Pop plot is 0.13 mm compared to the experimental value for the reaction zone width of about 0.025 mm at $\lambda = 0.90$; see [Menikoff, 2006] and [Gustavsen et al., 1998a,b]. The reaction zone width introduces a length scale and can be used as a shift in the origin in x. This helps to regularize the rate $\mathcal{R}(P)$ at $P_{\rm CJ}$ constructed in the next section.

Similarly, the time-to-detonation can be fit to straight line on log-log plot. In principle, distance-to-detonation and time-to-detonation determine $u_s(P)$ for a reactive shock. But the inaccuracy due to uncertainties in the measurements is severe. As an example, for PBX 9501 [Gibbs and Popolato,

1980, p. 115]

$$\log(P) = (1.10 \pm 0.04) - (0.51 \pm 0.03)\log(x) \ ,$$
$$\log(P) = (0.76 \pm 0.01) - (0.45 \pm 0.03)\log(t) \ .$$

It follows that $u_s = \frac{\mathsf{d}x}{\mathsf{d}t} = \frac{\mathsf{d}P/\mathsf{d}t}{\mathsf{d}P/\mathsf{d}x}$ can be expressed in terms of P as

$$u_s \propto P^{\left[\frac{1}{0.45\pm0.03} - \frac{1}{0.51\pm0.03}\right]} \propto P^{0.26\pm0.26} \ .$$

Clearly the uncertainty is too large for this expression to be useful.

Alternatively, the shock velocity can be determined from the x–t trajectory, and then using the single curve buildup principle associated with the shock pressure at the corresponding distance of run. In other words, $u_s(P)$ can be determined from the shock trajectory and the Pop plot. The shock relation, $P = P_0 + \rho_0 u_p u_s$, would then determine a self-consistent u_s–u_p relation for the Hugoniot locus of the reactive shock.

To illustrative these relations, we use the Hugoniot locus in fig. 1 and the Pop plot in fig. 5 to calculate the x–t trajectory for PBX 9501. For a linear u_s–u_p relation, the shock velocity in terms of the pressure is given by

$$u_s(P) = \tfrac{1}{2}\left(c_0 + \left[c_0^2 + 4s\,(P - P_0)\,V_0\right]^{1/2}\right) \ .$$

From Eq. (7) for the Pop plot, $P(x) = \frac{10^a}{x^b}$. Hence $u_s(P(x))$ determines the shock velocity as a function of distance. The corresponding time on the shock trajectory is

$$t(x) = t_{\mathrm{CJ}} + \int_0^x \frac{\mathsf{d}x}{u_s(x)} \ ,$$

where relative to the Pop plot x is replaced by $-x$. It is natural to take $t_{\mathrm{CJ}} = x_{\mathrm{CJ}}/D_{\mathrm{CJ}}$ where x_{CJ} is the distance of run on the Pop plot at the CJ pressure. The result, shown in fig. 6, is comparable to the measured trajectory in fig. 3. Also shown in fig. 6 is the reaction progress variable. The abrupt transition to detonation is due to the rapid change in λ as the reaction rate increases with shock pressure. This is the analog of an induction time for a homogeneous explosive with an Arrhenius rate.

The corresponding shock velocity and time-to-detonation for the model are shown in fig. 7. As with the standard Pop plot, time-to-detonation is nearly linear on a log-log scale. However, as discussed above, linear relations for both distance-to-detonation and time-to-detonation are not consistent with the shock velocity. Nevertheless, it can be seen that to a good approximation both variables may be treated as linear.

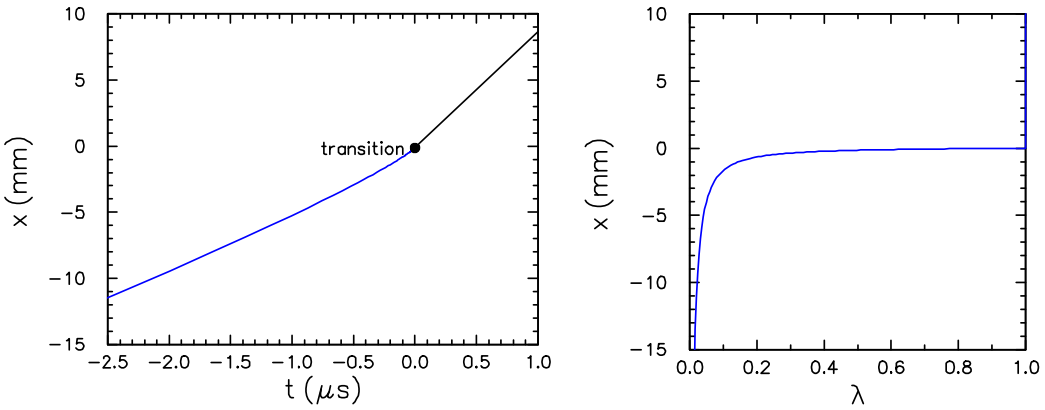
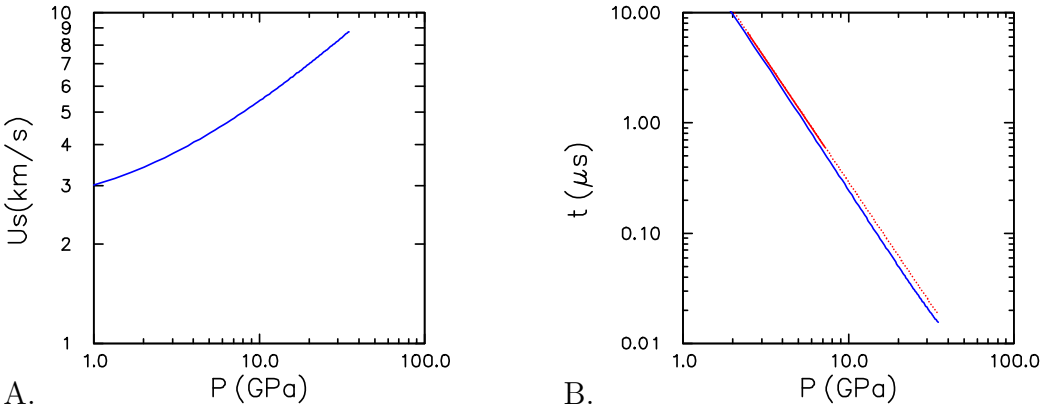


Figure 6: Shock trajectory for PBX 9501 computed from Hugoniot locus in fig. 1 and Pop plot in fig. 5.



A. B.

Figure 7: A. Shock velocity versus pressure on reactive Hugoniot locus shown in fig. 1. B. Blue curve is time-to-detonation corresponding to trajectory in fig. 6. Red curve is based on fit parameters from Gibbs and Popolato [1980, p. 115].

5 Reaction rate

The PDEs for reactive flow, Eq. (1), can be written in characteristic form; see Appendix A. The characteristic equations have source terms from the reaction rate. For the forward characteristic, Eq. (21a),

$$[\partial_t + (u+c)\partial_x]P + \rho c\,[\partial_t + (u+c)\partial_x]u = (\partial_\lambda P)\mathcal{R}\ ,$$

where ∂_λ is at fixed V and e. To apply this equation at the shock front, we decompose the characteristic derivative as

$$[\partial_t + (u+c)\partial_x] = [\partial_t + u_s\partial_x] + (u + c - u_s)\partial_x \ ,$$

and note that $\frac{\mathsf{d}}{\mathsf{d}t_s} = [\partial_t + u_s\partial_x]$ is the derivative along the shock front. Then the characteristic equation can be re-expressed as

$$\frac{\mathsf{d}}{\mathsf{d}t_s}P + \rho c\,\frac{\mathsf{d}}{\mathsf{d}t_s}u = (\partial_\lambda P)\mathcal{R} - \Big(u + c - u_s\Big)\Big(\partial_x P + \rho c\,\partial_x u\Big) \ . \tag{8}$$

A key approximation in the Forest fire model is to neglect gradients behind the front. We note that the gradient terms are proportional to $u + c - u_s$, and that this factor is small because the reactive locus is close to the partly burned CJ states; see fig. 1. Alternatively, the approximation can be thought of as having a rate sufficiently large to dominate the right hand side of Eq. (8). This is slightly different than the assumption in the original derivation [Mader and Forest, 1976] that $\partial_x P = 0$; see Appendix B.

When the gradients are neglected, the compatibility relation corresponding to the forward characteristic becomes

$$\frac{\Delta P}{\rho c^2} + \frac{\Delta u}{c} = \frac{\partial_\lambda P}{\rho c^2}\mathcal{R}\,\Delta t \ , \quad \text{along} \quad \Delta x = u_s \Delta t \ .$$

This can be re-expressed as

$$\frac{\mathsf{d}P_s/\mathsf{d}x}{\rho c^2} + \frac{\mathsf{d}u_p/\mathsf{d}x}{c} = \frac{\partial_\lambda P}{\rho c^2}\frac{\mathcal{R}}{u_s} \ , \tag{9}$$

where P_s and u_p are the pressure and particle velocity behind the reactive shock. Substituting $\mathsf{d}u_p/\mathsf{d}x = (\mathsf{d}P_s/\mathsf{d}x)/(\mathsf{d}P_s/\mathsf{d}u_p)$ and Eq. (6c) to eliminate the velocity derivative yields

$$\mathcal{R} = \left[1 + \frac{\frac{\rho\, c}{\rho_0 u_s}}{1 + \frac{u}{u_s}\,\frac{\mathsf{d}u_s}{\mathsf{d}u}}\right]\frac{u_s}{\partial_\lambda P}\,\frac{\mathsf{d}P_s}{\mathsf{d}x} \ . \tag{10}$$

The derivative $\mathsf{d}P_s/\mathsf{d}x$ is obtained from the Pop plot. Hence, the rate at the front is determined from the reactive Hugoniot and the Pop plot.

The reactive Hugoniot can be parameterized by the pressure. Utilizing Eq. (7) for the Pop plot,

$$\frac{\mathsf{d}P_s}{\mathsf{d}x} = -b\,\frac{P - P_\star}{x} = b\,10^{-a/b}\,(P - P_\star)^{1+1/b}. \tag{11}$$

Hence, $\mathcal{R}$ can be parameterized by the shock pressure. The Forest fire model assumes that there is a global rate of the form, Eq. (2),

$$\mathcal{R}(P,\lambda) = (1-\lambda)\mathcal{R}_{\mathrm{FF}}(P) \ ,$$

and fits the function $\mathcal{R}_{\mathrm{FF}}$ to the rate at the front.

We note that the rate $\mathcal{R}$ is proportional to $\mathsf{d}P_s/\mathsf{d}x$ and that the pressure derivative, Eq. (11), does not vanish at the CJ pressure. This is incompatible with the Eq. (2) since $\lambda = 1$ at $P = P_{\mathrm{CJ}}$. The inconsistency results in a singularity in $\mathcal{R}_{\mathrm{FF}}(P)$. The singularity is due in part to extrapolating the Pop plot and the fact that a first order rate gives rise to an exponential tail. In contrast, a rate proportional to $(1-\lambda)^n$ with $n < 1$ would lead to a finite reaction zone. The singularity could then be removed in a consistent manner by modifying the Pop plot. For example, one can take a transition distance x_1 such that the pressure on Pop plot corresponds to point on reactive shock locus with $\lambda = 0.95$, and then redefine distance of run for $x < x_1$ by

$$x = x_{\mathrm{CJ}} + A(P_{\mathrm{CJ}} - P)^{1-n} \ ,$$

where the parameters A and x_{CJ} are chosen such that $P(x)$ and $\mathsf{d}P/\mathsf{d}x$ are continuous at $x = x_1$. This has the effect of regularizing $\mathcal{R}_{\mathrm{FF}}$ near P_{CJ}. Other regularizations are discussed in sec. 6.1.

As an example, the Forest fire rate for PBX 9501 is shown in fig. 8. It has been regularized by the simple expediency of limiting λ to be less than 0.95. By construction, the Forest fire rate is restricted to pressures below the pressure at the CJ state. Moreover, since Pop plot data does not extend up to P_{CJ}, the Forest fire rate is not expected to be accurate near P_{CJ}.

We also note that the derived rate depends on the choice of EOS model. For example, the PBX 9501 rate shown in fig. 8 is about 3 times larger near the CJ pressure than the rate for PBX 9404 shown in [Mader, 1998, fig. 4.6, p. 199]. PBX 9404 has a similar high HMX content to PBX 9501, but is more sensitive at shock pressures below 10 GPa. The difference in the rates is partly due to the Pop plots shown in fig. 5 and partly due to the EOS models.

The measured reaction zone profile for PBX 9501 has the form of a classical ZND detonation [Gustavsen et al., 1998a,b]. Also shown in fig. 8 is the chemical rate based on reactant shock temperature from an EOS model and Arrhenius rate parameters compatible with the measured CJ wave profile [Menikoff, 2006]. We note that below the CJ pressure, the bulk chemical

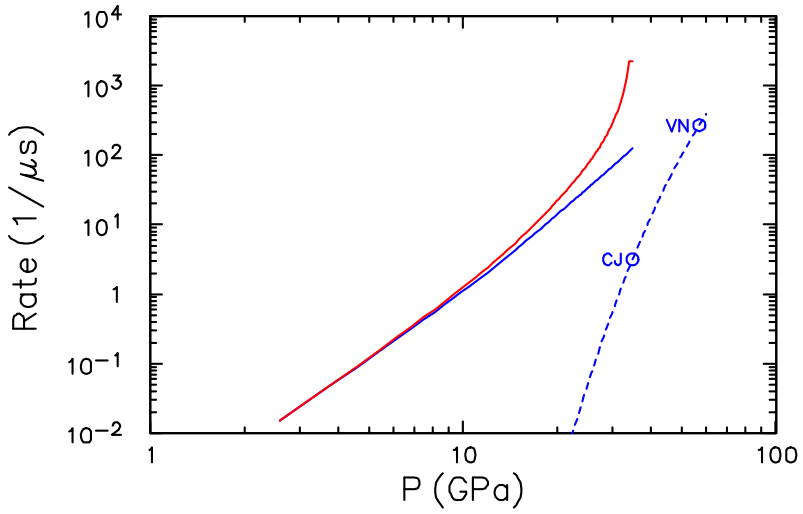


Figure 8: Forest fire rate for PBX 9501 using for distance of run-to-detonation $\log_{10}(P/\text{GPa}) = 1.10 - 0.51 \log_{10}(x/\text{mm})$ from Gibbs and Popolato [1980, p. 115]. Solid blue curve is $\mathcal{R}$ and red curve is $\mathcal{R}_{\text{FF}}$ with λ cutoff at 0.95 to avoid singularity. Dashed blue line is chemical rate based on reactant shock temperature and Arrhenius rate compatible with measured reaction zone profile for steady planar detonation wave. Circles denote bulk rate at shock pressure corresponding to the CJ and VN states.

rate is less than the Forest fire rate. This is an indication that reaction is dominated by hot spots. However, at the von Neumann (VN) spike state, the chemical reaction is sufficiently large to dominate a steady propagating detonation wave. In this regard, PBX 9501 may be an exceptional case because its high HMX content leads to a large detonation velocity and consequently the VN spike temperature is higher than for other PBXs. The increased detonation velocity has a large effect on the bulk rate since the chemical rate is very sensitive to temperature

In numerical simulations, as noted by Lunstrom [1988], the gradient behind the lead shock front becomes large as a detonation wave is approached. This is discussed further in a later section. Large gradients are also observed in velocity gauge data, see fig. 9. Consequently, the conceptual difference in the assumption on the forward characteristic used to derive the Forest fire rate — source term dominating versus a zero pressure gradient — is significant.

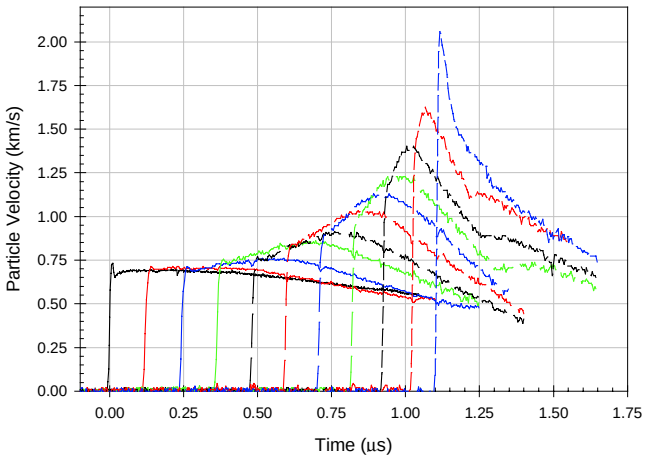


Figure 9: Lagrangian velocity time histories for shock initiation of PBX 9501 at input pressure of 5.15 GPa. The initial positions are 0.5 mm apart. Magnetic velocity gauge data is from Gustavsen et al. [1999, fig. 6]; reproduced with permission of the authors. The x–t trajectory for same experiment is shown in fig. 3.

We also note that by the last gauge in fig. 9, the wave has transited to a detonation. The peak velocity is nearly the same as the CJ state velocity (2.17 km/s) of PBX 9501 based on the EOS. Velocity Interferometry System for Any Reflector (VISAR) measurements with high temporal resolution (1 ns) show a VN spike velocity (3.55 km/s) matching that computed from the EOS [Gustavsen et al., 1998a,b, Fedorov, 2002, Menikoff, 2006]. The gauge record is an example in which limited resolution, from the response time of the gauge, gives the appearance of a reactive shock.

In principle, the gradient can be taken into account with an iterative scheme. Neglecting the gradients, as discussed above, can be consider as an initial approximation for the Forest fire rate $\mathcal{R}_{\text{FF}}$. This can be used in a numerical simulation of a shock-to-detonation transition to compute the gradients behind the front as a function of shock pressure. The gradients can then be incorporated in the characteristic equation and used to determine a better approximation for $\mathcal{R}_{\text{FF}}$. In practice this is not done. Though it may be important for insensitive explosives in which the rate does not totally dominate the behavior of the shock front. We conjecture that if the gradients are important for determining the rate then the single curve buildup principle would break down.

5.1 Shock dynamics

There is an interesting analogous to Whitham-Chisnell shock dynamics [see Whitham, 1974, sec. 8.1] for a shock wave propagating in a duct with variable cross sectional area. A source term arises in the characteristic equations from the change in area. Thus, $\mathsf{d}A/\mathsf{d}x$ plays a role analogous to the reaction rate. For duct flow, the source term is specified and the forward characteristic equation determines the shock strength as a function of area. The Forest fire model, on the other hand, uses the forward characteristic equation in the reverse manner; the shock strength is given and used to determine the source term, *i.e.*, the reaction rate.

Compared to the Guderley solution, shock dynamics is a very good approximation for a converging shock. This is because the converging shock front accelerates and outruns the interactions generated by the backward characteristic. Similarly, reaction accelerates a shock wave. Moreover, the state behind a reactive shock is approaching the sonic condition (CJ state) which would decouple the reaction zone from the flow behind. The Guderley solution has a limiting characteristic which plays an analogous role to the sonic condition for a detonation wave.

The exact Guderley solution requires that the far boundary condition is compatible with the similarity solution. However, independent of the boundary condition, a converging shock asymptotically approaches the portion of the Guderley solution between the shock front and the limiting characteristic. Very likely, the single curve buildup principle is an asymptotic approximation analogous to the Guderley solution for a converging shock. This provides some intuition as to why the Forest fire model works as well as it does.

6 Implementation issues

Key issues for implementing the Forest fire model are related to the singularity in the derived rate at the CJ pressure, and to the assumption of a reactive shock. These issues are discussed next.

6.1 Fitting form for rate

In the original Forest fire model, Mader and Forest [1976] fit $\ln[\mathcal{R}_{\mathrm{FF}}(P)]$ to a polynomial in P with up to 14 coefficients. We note from fig. 1B and fig. 8 that both λ and $\ln \mathcal{R}$ are smooth functions of P. In fact, $\mathcal{R}(P)$ is nearly linear

on a log-log plot. Hence, $\mathcal{R} \approx \text{constant} \times P^n$ with non-integer n. Rather than a high order polynomial, it would be better to fit λ and $\mathcal{R}/P^n$ separately to low order polynomials and express the Forest fire rate as a rational function

$$\mathcal{R}_{\text{FF}}(P) = \mathcal{R}(P)/[1 - \lambda(P)] \; . \tag{12}$$

Alternatively a cubic spline could be used to fit $\mathcal{R}_{\text{FF}}$. Splines are now a well developed method for approximating functions and efficient to evaluate.

At the CJ pressure, $\lambda = 1$, and Eq. (12) is singular. One way to regularize $\mathcal{R}_{\text{FF}}$ is to apply a cutoff; for example, to replace λ with $\min(0.95, \lambda)$. In fact, to avoid difficulties with incomplete burn, codes typically burn the remainder of any cell with λ above a cutoff of about 0.95; see for example [Mader, 1998, p. 197] or [Shaw and Straub, 1981, pp. 215–220].

Another way to regularize $\mathcal{R}_{\text{FF}}$ is to modify the reactive Hugoniot locus such that the CJ pressure corresponds to a smaller wave speed than the CJ detonation speed. For a linear u_s–u_p relation, this amount to using a smaller value of s than $(D_{\text{CJ}} - c_0)/u_{\text{CJ}}$, which results in a higher compression ratio for a given shock pressure. Combined with extending the Pop plot and applying Eq. (10), the rate can be extended slightly beyond P_{CJ}. It is important to note that neither Hugoniot data nor Pop-plot data extend up to the CJ pressure. Therefore, any regularization is necessarily ad hoc.

We note that the factor $1 - \lambda$ in Eq. (2) would correspond to a first order reaction for a homogeneous material. For a heterogeneous explosive, the reaction rate is due to hot spots, and an ignition and growth burn mechanism is plausible. In this case, reaction is dominated by deflagration fronts triggered by hot spots. The dependence of the rate on the reaction progress variable can then be associated with the area of the burn front; for example, $\lambda^{2/3}$ for outward hole burning or $(1 - \lambda)^{2/3}$ for inward grain burning. This modification to the Forest fire rate has been suggested by Starkenberg [1993, p. 999]. We note that the exponent for grain burning is less than 1. Consequently, a steady wave would have a finite reaction zone width. This is in contrast to a first order reaction which has an exponential tail.

6.2 Reactive shock profile

The Forest fire model was developed and has been used in hydro codes with a shock capturing algorithm based on artificial viscosity. Rather than a discontinuous reactive shock, burning occurs within the numerical shock profile. In

contrast to a ZND wave profile, a steady detonation wave for the Forest fire model has a continuous profile usually associated with a weak detonation. A continuous profile is an implicit requirement of the Forest fire model since the derivation of the rate only extends up to the CJ pressure.

The standard operating procedure for simulations with the Forest fire model is to tune the viscous coefficient on the grid being used such that a planar steady detonation wave profile ends at the CJ state rather than a point on the weak branch of the detonation locus. In addition, for Lagrangian algorithms, the reaction rate is typically taken to be a function of the sum of the pressure + the viscous pressure; see for example, [Shaw and Straub, 1981, p. 219]. This has two important consequences. First, the model depends on the form of the numerical dissipation used for shock capturing, and hence the solution is implementation dependent. Second, the viscosity must be adjusted with the cell size in order for the solution to converge under mesh refinement. Since the choice of the viscous coefficient is imprecise, convergence studies would be somewhat subjective.

In addition, the Forest fire model was developed in the 1970s when the available computing power limited the mesh resolution that could be used. The cell size, in effect, introduced a length scale which can have a significant effect on the results of a simulations. In order for the Forest fire model to be well posed, the dissipation required for the detonation profile needs to be included as an integral part of the model. We suggest utilizing a viscous pressure analogous to the von Neumann-Richtmyer artificial viscosity. Namely, to replace P in Eq. (1) with $P + Q$, and choose for the viscous pressure

$$Q = -\nu\rho \left[c + r \left| \ell \frac{\mathsf{d}u}{\mathsf{d}x} \right| \right] \ell \frac{\mathsf{d}u}{\mathsf{d}x} \ , \tag{13}$$

where ν is a dimensionless viscous coefficient, r is the ratio of quadratic to linear viscous terms, and ℓ is a length scale.

The continuum mechanics viscosity can be reduced to the usual form of numerical artificial viscosity by taking ℓ to be the cell size and replacing $\ell \frac{\mathsf{d}u}{\mathsf{d}x}$ with Δu, *i.e.*, the velocity difference across a cell.[5] The effective coefficient

[5]Modern shock capturing algorithms aim at minimizing the number of cells in the numerical shock profile. One method for Eulerian algorithms is to construct a piecewise linear velocity from the values of velocity at the cell centers, then to replace Δu in the formula for Q by the discontinuity at the cell boundary. Alternatively, numerical dissipation can be introduced using approximate Riemann solvers for the flux at cell boundary, rather than with a viscous pressure.

of dynamic viscosity[6] is proportional to $\nu\,\rho\,c\,\ell$. For an artificial viscosity, it decreases with grid resolution. In contrast, our motivation for using Eq. (13) is to introduce a length scale in the continuum equations for the model, and relate ℓ to the reaction zone width independent of the grid size.

6.2.1 Detonation wave profile

It is instructive to analyze the detonation wave profile for the continuum PDEs. The general case, with viscosity, heat conduction and mass diffusion has been worked out; see Gasser and Szmolyan [1993] and references therein to earlier work. The problem is much easier when only viscosity is considered. Then the problem can be reduced to a system of only two ODE and the phase plane can be readily visualized.

For a steady planar detonation wave with Eq. (13) for the viscous pressure, the wave profile is determined by the ODEs

$$\begin{aligned} \frac{\mathsf{d}}{\mathsf{d}\xi} u &= -\frac{c}{2\,r\,\ell}\left[\left(1+4r\left|\frac{Q}{\nu\,\rho\,c^2}\right|\right)^{1/2}-1\right]\mathsf{sgn}(Q)\ , \\ \frac{\mathsf{d}}{\mathsf{d}\xi}\lambda &= -\frac{\mathcal{R}(\lambda,P+Q)}{D-u}\ , \end{aligned} \tag{14}$$

where $\xi = x - D\,t$ is spatial coordinate, and D is the wave speed. The other variables are obtained from algebraic equations:

$$\begin{aligned} V &= V_0 - u/m\ , \\ e &= e_0 + (P_0/m + \tfrac{1}{2}u)\,u\ , \\ P &= P(V,e,\lambda)\ , \\ Q &= m\,u - P + P_0\ , \end{aligned}$$

where $m = \rho_0(D-u)$ is the mass flux. The initial state, at $\xi = \infty$, is denoted by subscript '0'.

In the (u,λ) phase plane, the weak and strong points on the detonation locus and the initial state[7] are fixed points for which the right hand side of Eq. (14) vanishes. The locus in the phase plane corresponding to the

[6] Dynamic viscosity has units of pressure × time.

[7] To avoid the so called hot boundary problem, we assume a small cutoff pressure below which the rate vanishes. This is equivalent to assuming that the trajectory for the wave profile at the initial state has slope $\mathsf{d}\lambda/\mathsf{d}u = 0$.

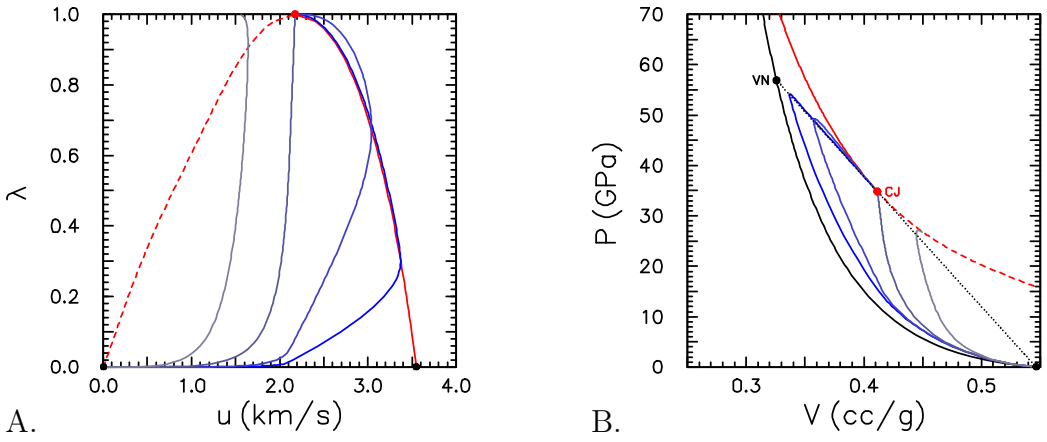


Figure 10: Phase plane for steady viscous detonation wave in PBX 9501 at CJ wave speed. Trajectories shown for viscosity of $\nu = 0.001$, 0.01, 0.35, 5 (varying with blue tint). Dashed line does not end at fixed point and hence does not correspond to steady profile. A. Red curve is image of Rayleigh line; dashed and solid are weak and strong branch, respectively. B. Black curve is unreacted shock locus, and red curve is detonation locus; dashed and solid are weak and strong branch, respectively. Dotted black line is Rayleigh line. Red and black symbols denote CJ and von Neumann spike states, shock.

intersection in the (V, P)–plane of the Rayleigh line with the weak and strong points on the partially burned Hugoniot loci plays a key role. We observe that on the Rayleigh line $Q = 0$, and hence $\frac{du}{d\lambda} = 0$. It follows that $\frac{du}{d\lambda} > 0$ if and only if the state is between the weak and strong loci. As a consequence, the strong point on the detonation locus is a stable fixed point and the weak point is a saddle point. At the CJ detonation speed, the weak and strong points coincide. As a fixed point, the CJ state is stable for trajectories approaching from high pressure and unstable when trajectories approach from low pressure.

Example trajectories in the (u, λ)–plane and (V, P)–plane for PBX 9501 at CJ wave speed, as the viscosity coefficient ν is varied (with $\ell = 0.05\,\mathrm{mm}$ and $r = 0.5$), are shown in fig. 10. The trajectories vary with viscosity as follows:

(i) For small viscosity, there is a viscous shock profile to nearly the von Neumann spike state, followed by reaction along the Rayleigh line to the CJ state. This corresponds to the ZND profile.

(ii) For larger values of the viscosity, there is a competition between viscous

and reactive time scales that results in a non-monotonic profile with peak pressure below the von Neumann spike pressure.
(iii) There is a unique value of the viscous coefficient such that the pressure within the wave profile to the CJ state is monotonic. It is natural to base the Forest fire model on this value for the viscosity.
(iv) For still larger values of the viscous coefficient, the trajectory crosses the weak branch of the Rayleigh line and does not end on the detonation locus. These trajectories are not valid steady state profiles. The solution to the time dependent PDEs for an underdriven wave, would have a lower detonation speed for which the detonation profile would end on the weak branch of the detonation locus.

The unique CJ detonation wave profile with a monotonic pressure is shown for PBX 9501 in fig. 11. The reaction zone width is an important quantity. To avoid the precursor tail we take the spatial origin — somewhat arbitrarily — to correspond to a pressure of 0.1 GPa. We note that the viscous pressure at the spatial origin is much larger, order of 1 GPa. With this choice, the width of the reaction zone for the Forest fire model is about 0.05 mm. This is comparable to the experimental value of 0.025 mm based on VISAR measurements; see [Menikoff, 2006] and references therein. For the Pop plot, on which the rate is based, the run distance at the CJ pressure is 0.13 mm. The model reaction width can be varied with the form of the viscous pressure, such as parameter r in Eq. (13), or with the reaction order for the rate. This freedom can be used to adjust the magnitude of the curvature effect discussed in sec. 8.2.

Several remarks are in order:
(i) The Pop plot does not determine the steady reaction zone width. The extrapolated distance of run at CJ pressure only gives an indication of a relevant length scale for the Forest fire model. For a reactive shock, the width would literally be zero. The actual width reflects an inconsistency between the reactive shock assumption and the implementation of the model with a continuous profile. Moreover, a shock capturing scheme can not distinguish the reaction in the shock profile from subsequent reaction that accelerates a reactive shock to a detonation wave. Because of the inconsistency between the assumption and implementation, the model will not reproduce the Pop plot exactly.
(ii) The viscous pressure Q peaks at $\lambda \approx 4\,\%$. Reaction in the shock rise is enhance by taking the rate to be a function of $P + Q$, and is in keeping with the assumption of a reactive shock. If instead the rate in Eq. (14) is taken

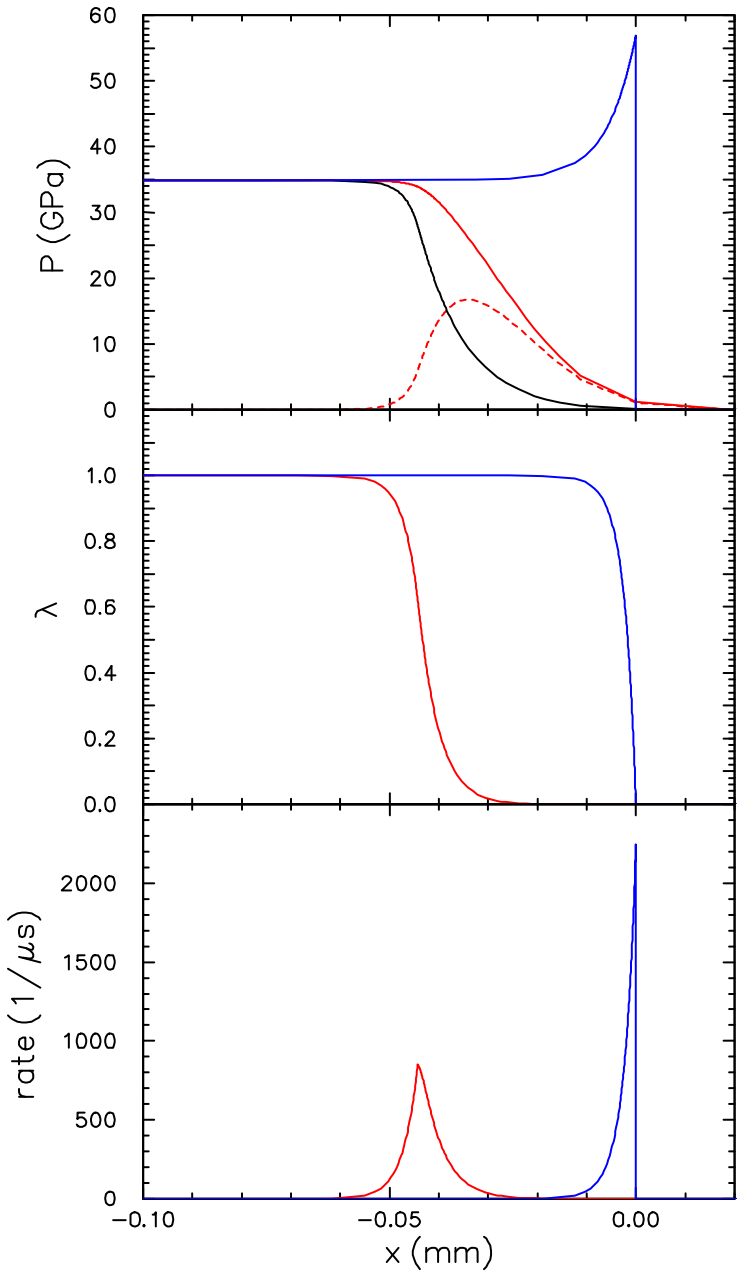


Figure 11: Detonation wave profile for PBX 9501. Red and blue curves correspond to Forest fire rate with viscous shock and discontinuous lead shock, respectively. For viscous profiles, spatial origin corresponds to pressure of 0.1 GPa. For the pressure plot, black, red and dashed red curves are P, $P + Q$ and Q, respectively.

as a function of P, then the viscous coefficient needed for the unique monotonic detonation profile would be over an order of magnitude larger and the reaction zone width in excess of 1 mm. We note that the advection step in an Eulerian simulation is diffusive, and some implementations of the Forest fire model do use a rate as a function of P rather than $P + Q$.
(iii) Suppose one were to use only an artificial viscosity with fixed value of viscous coefficient. Then as the mesh is refined and the effective viscous coefficient decreased, the reaction zone profile would approach the ZND profile; blue curve in fig. 11. On the other hand, suppose both an artificial and continuum form of viscous pressure were used. Then on coarse meshes the artificial viscosity would dominate and a simulation would be similar to present implementations. But on fine meshes, when Eq. (13) dominates, the solution should converge to the continuum solution with the steady profile shown in fig. 11. It is important to note that when the continuum Q dominates the reaction zone, the PDEs would have a parabolic character. The stability criterion for an explicit algorithm would then be $\Delta t < (\Delta x)^2/(\nu\, c\, \ell)$ rather than the hyperbolic CFL condition, $\Delta t < \Delta x/c$. Consequently, either very small time steps or an implicit algorithm, such as backward Euler, would be needed on very fine meshes.

Other forms of numerical dissipation have been used for shock capturing algorithms. In particular, Godonov algorithms use approximate Riemann solvers. On coarse meshes with a fast reaction rate, weak detonation waves with continuous profiles can occur in simulations; see Colella et al. [1986]. In contrast to artificial viscosity methods, the dissipation in a Godunov algorithm can be increased only a limited amount by reducing the scheme to first order. Consequently, under mesh resolution the solution for a steady detonation wave would converge to a ZND profile. Thus the original Forest fire model could only be applied with a Godonov scheme on coarse meshes. Explicitly, introducing a viscous dissipation into the Forest fire model enables the model to be well posed independent of the numerical dissipation used by a shock capturing algorithm.

Finally, we note that Starkenberg [1993] implemented the Forest fire model in a 1-D code with a true reactive shock by tracking the lead front. Tracking is considerably more difficult in 2-D. In addition, there are issues with multiple shocks and the curvature effect, discussed in the next section, which would be difficult to overcome with front tracking.

7 Numerical example

To illustrate some of the properties of the Forest fire model we have run a shock-to-detonation simulation for PBX 9501. The calculation uses a Godunov algorithm with the continuum viscosity described in the previous section. The viscous reactive profile is resolved with an adaptive mesh. The shock is driven by a piston with velocity of 0.7 km/s. This case corresponds to the gas gun experiment by Gustavsen et al. [1999] with shock trajectory and velocity gauge data shown in figs. 3 and 9.

The time evolution of pressure, particle velocity and burn fraction are shown in fig. 12. Several features of the profiles are noteworthy: (i) Though the reaction zone profile is resolved numerically (finest grid with 5 μm cell size), on the 10 mm scale of the plot, the lead wave appears discontinuous. (ii) The pressure gradient behind the lead shock is fairly small up to pressures of about 15 GPa. But at higher pressures, there is a significant gradient. Moreover, the sign of the gradient is such as would weaken a shock in an inert flow. The rapid increase in shock pressure implies that the reactive source term dominates over the gradients for the transition to detonation. (iii) The rapid final stage of the transition to detonation is a transient. At the transition, the shock pressure exceeds the CJ pressure and then on the time scale of the reaction zone (10 ns) equilibrates to the CJ pressure. The pressure spike gives rise to a left facing wave seen in the subsequent pressure and velocity profiles. (iv) Even for relatively weak shocks, there is a significant gradient in the particle velocity. The velocity gradient is a consequence of the shock acceleration, *i.e.*, the shock-change equation described in Appendix B.

Lagrangian velocity time histories are shown in fig. 13. We note that Lagrangian time histories are considerably different than the profiles at fixed time. Only for a steady wave would they be the same, up to a scale factor of the axes; $x/t = D$. Compared to the experimental measurement shown in fig. 9, shock arrival times at the gauges are in good agreement, because the model is calibrated to the Pop plot. But the shape of the profiles clearly differ. The velocity at late time is affected by the boundary condition. The piston boundary does not allow the explosive to expand against the experimental flyer plate as the pressure rises due to reaction. In addition, the gauges perturb the flow. Nevertheless, the difference behind the shock front is larger than the expected experimental uncertainty.

This example illustrates a strength and weakness of the Forest fire model. An advantage of the model is that only limited data — Pop plot and reactive

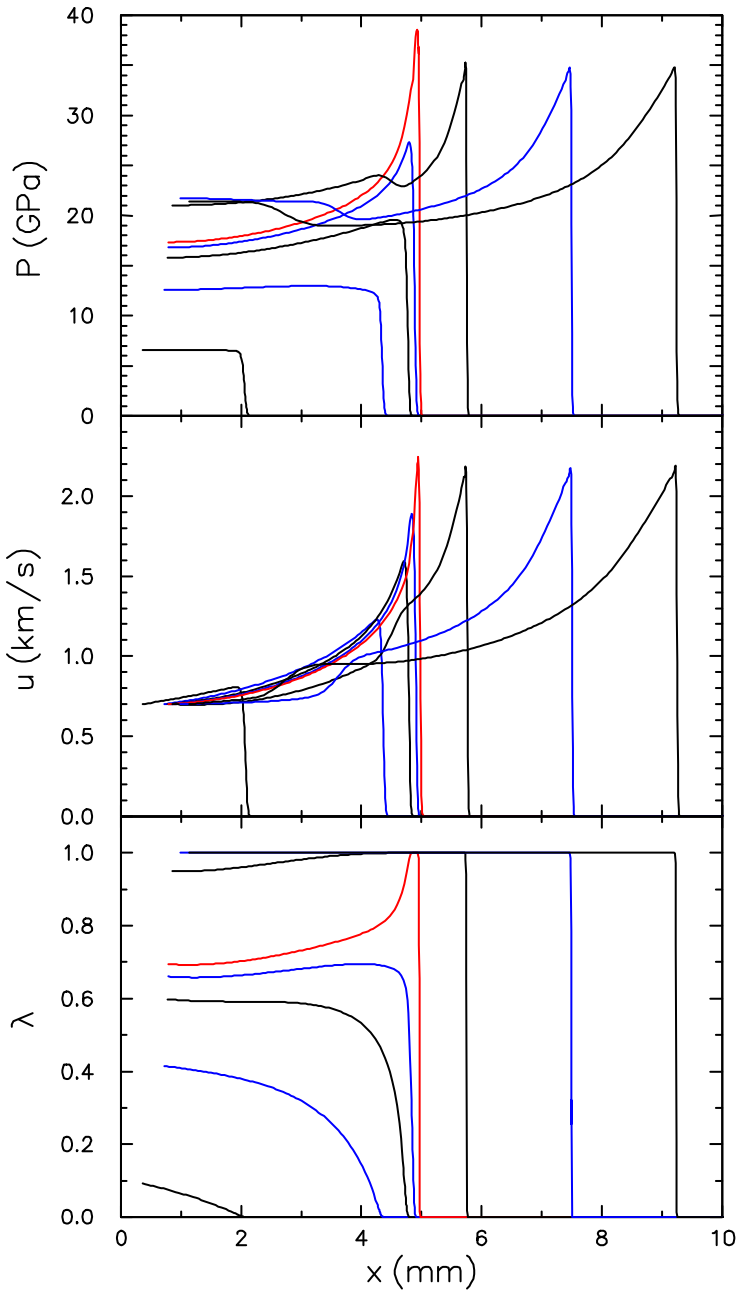


Figure 12: Evolution of P, u and λ profiles for shock-to-detonation transition in PBX 9501. Profiles are at $t = 0.5, 1.0, 1.08, 1.1, 1.11, 1.2, 1.4, 1.6\,\mu$s. Transition at $t = 1.11\,\mu$s is shown as red curve in each plot.

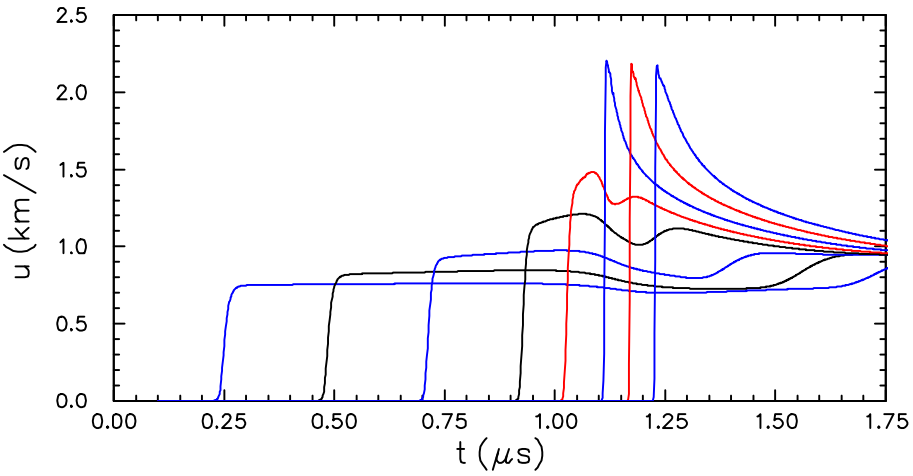


Figure 13: Simulated Lagrangian velocity time histories for shock-to-detonation transition in PBX 9501. The initial positions are at $x_0 = 1, 2, 3, 4, 4.5, 5, 5.5, 6$ mm.

Hugoniot — is needed to calibrate the rate. The flip side is that the model has no degrees of freedom to fit profile data empirically. Based on the simplifying model assumption, that the global rate has the same functional form as it does at the front, there is no reason to expect good agreement with profile data which is affected by the rate behind the front.

8 Model limitations

Simplified burn models have their limitations. Inaccuracies result from tacit assumptions on the hot-spot distribution and an overly large reaction zone width from lack of resolution. These points are briefly discussed next.

8.1 Shock desensitization

The Forest fire rate is calibrated to Pop-plot data, *i.e.*, shock-to-detonation transition experiments. Hence it assumes a hot-spot distribution from a single shock. Other experiments demonstrate that the hot-spot distribution is affected by the flow. A notable example is shock desensitization, in which a weak shock can quench a propagating detonation wave [Campbell and Travis, 1986]. For a PBX, ignition is sensitive to small amounts of porosity.

Presumably, a weak shock can close pores and eliminate potential nucleation sites for hot spots from subsequent waves. A rate that depends only on pressure, can not account for this effect.

Simple burn models can be extended by adding another variable to keep track of the lead shock strength as a function of position, and then adjusting the rate based on the lead shock strength. One such model is multiple-shock Forest fire, see [Mader, 1998, sec. 4.3] and [Mader et al., 2002]. An algorithm for a shock pressure variable can be based on the artificial viscous pressure which peaks within a numerical shock profile. The Forest fire rate is then limited to a value corresponding to the lead shock pressure. In effect, the rate is a function of an additional internal state variable; $\mathcal{R}(\lambda, P, P_s)$. For a more detailed discussion of burn models motivated by hot spots and the dependence of the burn rate on lead shock pressure see Johnson, Tang, and Forest [1985], in particular, their discussion around Eqs. (19) and (20).

Several other experiments show that the flow affects the hot-spot distribution, and hence the rate. Noteworthy is the 2-D flow that arises from detonation diffraction, often referred to as corner turning, which leads to a pocket of unreacted HE called a dead zone. Pressure dependent rates alone are not sufficient to reproduce dead zones; see DeOliveria et al. [2006] and references therein.

Isentropic compression techniques have been developed for high pressure equation of state measurements; see [Hooks et al., 2006, Baer et al., 2006]. Due to the absence of dissipation from shock heating, isentropic compression would generate fewer and weaker hot spots than shock compression to the same pressure. Consequently, the Forest fire rate would overpredict the reaction rate for isentropic compression, or more generally when a ramp pressure rather than a shock is applied to an HE; see Starkenberg [1993].

8.2 Curvature effect

Though the CJ detonation velocity is the minimum wave speed for a planar detonation wave, rate stick experiments [Campbell and Engelke, 1976] have shown that curved detonation waves have a lower detonation velocity. Donguy and Legrand [1981] have performed simulations of rate sticks with the Forest fire model and compared with experiments using a PBX composed of 95.5 wt % TATB and 4.5 wt % VITON. They find on coarse meshes that the simulations display a large diameter effect; variation of detonation velocity with rate stick diameter. Moreover, the numerical diameter effect

appears to converge to the experimental measurements as the mesh is refined. They do not, however, specify the form of artificial viscosity used or how the viscous coefficient is adjusted with mesh size.

Over predicting the diameter effect is a generic problem for simulations when the reaction zone is not sufficiently resolved. It can be explained as follows. The reaction zone width and front curvature together lead to modified jump conditions for a quasi-steady detonation wave, see Menikoff et al. [1996, Eq. (5.1–3)]:

$$\begin{aligned} \Delta[\rho(D-u)] &= \kappa w \, \langle \rho u \rangle \ , \\ \Delta \left[\Big(\rho(D-u) \Big)^2 V + P \right] &= \kappa w \, \langle \rho(D-u) u \rangle \ , \\ \Delta \left[E + PV + \tfrac{1}{2}(D-u)^2 \right] &= 0 \ , \end{aligned} \tag{15}$$

where $\Delta[f] = f(x_0) - f(x_1)$ is the change of variable f across the detonation wave, $w = x_0 - x_1$ is the reaction zone width, κ is the front curvature, and $\langle f \rangle = w^{-1} \int_{x_1}^{x_0} dx \, f$ is the average value of f in the reaction zone. For a planar front, $\kappa = 0$ and Eq. (15) reduces to the standard Rankine-Hugoniot jump conditions. On a coarse mesh, the reaction zone is not resolved and the reaction zone width will be artificially large. Since the right hand side of the jump conditions, Eq. (15), is proportional to κw, a conservative scheme can not distinguish between an artificially large w and a large κ, and therefore will over predict the effect of curvature.

We note that the right hand side of Eq. (15) is also proportional to average quantities within the reaction zone. Compared to other burn models with a ZND reaction zone profile, the average quantities will be lower for the Forest fire model since the density ρ increases monotonically from the initial state rather than decreasing monotonically from the von Neumann spike state. The smaller average quantities can compensate for a larger reaction zone width. Thus, the Forest fire model can give rise to the same curvature effect as other models having a smaller reaction zone width.

Two additional points are worth noting. First, a tracked reactive shock, as Starkenberg [1993] implemented in a 1-D code, would have a zero reaction zone width and hence the conservation laws would imply the absence of a curvature effect. Possibly, the curvature effect could be obtained utilizing a partly resolved reaction zone [Bdzil and Davis, 1975] in which the tracked reactive shock models a fast reaction for the bulk of the burn fraction and then the final slow reaction for the remainder of the burn fraction

is resolved. Second, for just propagation of a detonation wave, the Detonation Shock Dynamics (DSD) model can be used [Bdzil and Stewart, 1989, Aslam et al., 1996]. The model incorporates the curvature effect; detonation velocity as a function of local front curvature, $D(\kappa)$. Since DSD assumes a quasi-steady detonation wave, it is not suitable for initiation problems, which are inherently transient in nature.

9 Concluding remarks

Compared to other burn models, a distinguishing property of the Forest fire model is that the reaction zone for a steady detonation has a continuous profile, usually associated with a weak detonation, rather than a ZND profile. Since the Forest fire model is aimed at solid explosives, in particular plastic-bonded explosives, one might expect that the detonation front would be irregular due to heterogeneities within the explosive, and a homogenization based on averaging hydrodynamic variables transverse to the direction of wave propagation to give a smooth profile.

Some experiments do show front irregularities from hot spots, see for example [Plaksin et al., 2002] and references therein. Other experiments have measured the reaction zone of high HMX content PBXs, such as PBX 9501, using a velocity interferometry technique [Gustavsen et al., 1998a,b, Fedorov, 2002]. Their data displays a ZND profile which is compatible with an Arrhenius reaction rate based on bulk shock heating [Menikoff, 2006]. However, the spot size for the high resolution measurements is a fraction of a mm or a few times the average grain size. Other experimental techniques using the light intensity from a shock front [Loboiko and Lubyatinsky, 2000] give information on the average behavior of the reaction zone. However, the nature of the averaging is not clear. Determination of a homogenized or average profile would require high resolution data (1 ns temporal resolution and 10 μm spatial resolution) over a mm wide region of the detonation front. Until such data becomes available, despite the derivation for the reaction rate, Forest fire should be regarded as an empirical model.

The Forest fire rate is calibrated to Pop-plot data or shock initiation experiments on distance-of-run to detonation. Other empirical models can fit Pop-plot data; see for example [Starkenberg et al., 2006]. To objectively compare Forest fire with other models, one first has to eliminate the implementation dependence. To this end we proposed in sec. 6.2 incorporating

a dissipative mechanism needed to get a well defined reaction zone profile directly in the Forest fire model.

Comparisons among models should also be done with mesh converged solutions. Coarse mesh solutions are of practical importance, but the mesh size needed for a desired accuracy should be a separate issue. However, resolution and model predictions may be coupled if model parameters are empirically fit based on coarse mesh solutions. As discussed in sec. 8.2, the numerical reaction zone width affects propagation of curved detonation waves. The steady CJ reaction zone width of a model is the critical length scale for setting the numerical resolution.

Finally, we note that the Pop plot for a given explosive depends on the initial temperature since an explosive is more sensitive when hot than cold. Simple burn models can not account for such changes in sensitivity. Typically, different rate calibrations are used for a hot and cold explosive. In effect, a hot and a cold explosive of the same material are modelled as different explosives. Similarly, a PBX is more sensitive when pressed to low density than to high density. The variation of the Pop plot with pressing density has been analyzed by Forest [1978]. Different Pop plots could also be used for a precompressed PBX to describe shock desensitization. On the other hand, damage can introduce porosity and sensitize a PBX. One needs to be cognizant of these limitation when using a model to predict the behavior of an explosive for a new application. This is particularly relevant to accident scenarios since an explosive can be subjected to a wider variety of initiation stimuli over longer time scales than the design mode for which model parameters are calibrated.

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Appendix A. Characteristic equations

The first step in deriving the characteristic equations for reactive flow is to re-express Eq. (1) in Lagrangian form:

$$\frac{\mathsf{d}V}{\mathsf{d}t} - V\partial_x u = 0 \ , \tag{16a}$$

$$\frac{\mathsf{d}u}{\mathsf{d}t} + V\partial_x P = 0 \ , \tag{16b}$$

$$\frac{\mathsf{d}e}{\mathsf{d}t} + PV\partial_x u = 0 \ , \tag{16c}$$

$$\frac{\mathsf{d}\lambda}{\mathsf{d}t} = \mathcal{R} \ , \tag{16d}$$

where $\frac{\mathsf{d}}{\mathsf{d}t} = \partial_t + u\partial_x$ is the convective time derivative. From Eq. (16a) and Eq. (16c), the energy equation can be express as

$$\frac{\mathsf{d}e}{\mathsf{d}t} + P\frac{\mathsf{d}V}{\mathsf{d}t} = 0 \ . \tag{17}$$

For a pressure-temperature equilibrium EOS, the mixture entropy is

$$S = \lambda_1 S_1 + \lambda_2 S_2 \ ,$$

and the fundamental thermodynamic identity in differential form is

$$\mathsf{d}e = -P\,\mathsf{d}V + T\,\mathsf{d}S - T\Delta S\,\mathsf{d}\lambda \ , \tag{18}$$

where $\Delta S = S_2 - S_1$ and the subscripts 1 and 2 denote the reactants and products, respectively. Substituting into Eq. (17) leads to the entropy equation

$$\frac{\mathsf{d}S}{\mathsf{d}t} = \Delta S\frac{\mathsf{d}\lambda}{\mathsf{d}t} = (\Delta S)\,\mathcal{R} \ . \tag{19}$$

Both the entropy equation (19) and the reaction equation (16d) are in characteristic form.

To obtain the acoustic characteristics, we begin by transforming the independent thermodynamic variables from (ρ, S) to (P, S). In differential form,

$$\mathsf{d}P = c^2\,\mathsf{d}\rho + (\partial_S P)_{V,\lambda}\,\mathsf{d}S + (\partial_\lambda P)_{S,\lambda}\,\mathsf{d}\lambda \ ,$$

where $c^2 = (\partial_\rho P)_{S,\lambda}$ is the square of the frozen sound speed. Utilizing Eq. (19), the time derivative of the pressure is

$$\frac{\mathsf{d}P}{\mathsf{d}t} = c^2 \frac{\mathsf{d}\rho}{\mathsf{d}t} + \Big[(\partial_S P)_{V,\lambda}\,\Delta S + (\partial_\lambda P)_{V,S}\Big] \frac{\mathsf{d}\lambda}{\mathsf{d}t} \ .$$

From Eq. (18), it can be shown that the term in square brackets is equal to $(\partial_\lambda P)_{V,e}$. Therefore,

$$\frac{\mathsf{d}P}{\mathsf{d}t} = c^2 \frac{\mathsf{d}\rho}{\mathsf{d}t} + (\partial_\lambda P)_{V,e}\mathcal{R} \ .$$

Utilizing Eq. (16a) to eliminate the derivative of ρ, we obtain

$$\frac{\mathsf{d}P}{\mathsf{d}t} + \rho c^2\,\partial_x u = (\partial_\lambda P)_{V,e}\mathcal{R} \ . \tag{20}$$

Linear combinations of Eq. (16b) and Eq. (20) lead to the characteristic equations for the acoustic modes:

$$\Big(\mathsf{d}/\mathsf{d}t + c\,\partial_x\Big)P + \rho c\Big(\mathsf{d}/\mathsf{d}t + c\,\partial_x\Big)u = (\partial_\lambda P)_{V,e}\mathcal{R} \ , \tag{21a}$$

$$\Big(\mathsf{d}/\mathsf{d}t - c\,\partial_x\Big)P - \rho c\Big(\mathsf{d}/\mathsf{d}t - c\,\partial_x\Big)u = (\partial_\lambda P)_{V,e}\mathcal{R} \ . \tag{21b}$$

Appendix B. Shock-change equation

Gradients in the flow variables behind a reactive shock can be related to the change in strength of the shock and the reaction rate. We start with the Lagrangian form of the flow equations (16b–d) and Eq. (20) substituted for the mass equation (16a). The time derivative along the front is

$$\frac{\mathsf{d}}{\mathsf{d}t_s} = \frac{\mathsf{d}}{\mathsf{d}t} + (u_s - u)\partial_x \ .$$

Substituting $\mathsf{d}/\mathsf{d}t_s$ for $\mathsf{d}/\mathsf{d}t$, the flow equations yield a system of linear equations for the flow gradients;

$$\begin{pmatrix} u_s-u & -\rho c^2 & 0 & 0 \\ -V & u_s-u & 0 & 0 \\ 0 & -PV & u_s-u & 0 \\ 0 & 0 & 0 & u_s-u \end{pmatrix} \begin{pmatrix} \partial_x P \\ \partial_x u \\ \partial_x e \\ \partial_x \lambda \end{pmatrix} = \begin{pmatrix} \frac{\mathsf{d}}{\mathsf{d}t_s}P - (\partial_\lambda P)_{V,e}\mathcal{R} \\ \frac{\mathsf{d}}{\mathsf{d}t_s}u \\ \frac{\mathsf{d}}{\mathsf{d}t_s}e \\ \frac{\mathsf{d}}{\mathsf{d}t_s}\lambda - \mathcal{R} \end{pmatrix} \ .$$

The matrix on the left hand side can be inverted to yield

$$\begin{pmatrix} \partial_x P \\ \partial_x u \\ \partial_x e \\ \partial_x \lambda \end{pmatrix} = \begin{pmatrix} -\frac{u_s-u}{w^2} & -\frac{\rho c^2}{w^2} & 0 & 0 \\ -\frac{V}{w^2} & -\frac{u_s-u}{w^2} & 0 & 0 \\ \frac{-PV^2}{(u_s-u)w^2} & -\frac{PV}{w^2} & \frac{1}{u_s-u} & 0 \\ 0 & 0 & 0 & \frac{1}{u_s-u} \end{pmatrix} \begin{pmatrix} \frac{\mathsf{d}}{\mathsf{d}t_s} P - (\partial_\lambda P)_{V,e} \mathcal{R} \\ \frac{\mathsf{d}}{\mathsf{d}t_s} u \\ \frac{\mathsf{d}}{\mathsf{d}t_s} e \\ \frac{\mathsf{d}}{\mathsf{d}t_s} \lambda - \mathcal{R} \end{pmatrix} , \quad (22)$$

where $w^2 = c^2 - (u_s - u)^2$.

For a shock-to-detonation transition, the time derivatives at the shock front are determined by the Pop plot and the reactive Hugoniot. There are 4 equations for 5 unknowns; 4 gradients and the rate. Hence the Forest fire model requires an additional assumption to determine the rate. For the original derivation [Mader and Forest, 1976], the assumption is that $\partial_x P = 0$. In this case

$$(\partial_\lambda P)\mathcal{R} = \frac{\mathsf{d}}{\mathsf{d}t_s} P + \frac{\rho c^2}{u_s - u} \frac{\mathsf{d}}{\mathsf{d}t_s} u \ .$$

The rate based on the forward characteristic, Eq. (9),

$$(\partial_\lambda P)\mathcal{R} = \frac{\mathsf{d}}{\mathsf{d}t_s} P + \rho c \frac{\mathsf{d}}{\mathsf{d}t_s} u \ ,$$

is slightly different.

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